QMCPACK

Overview, Features, Applications

Paul Kent (ORNL)

Outline

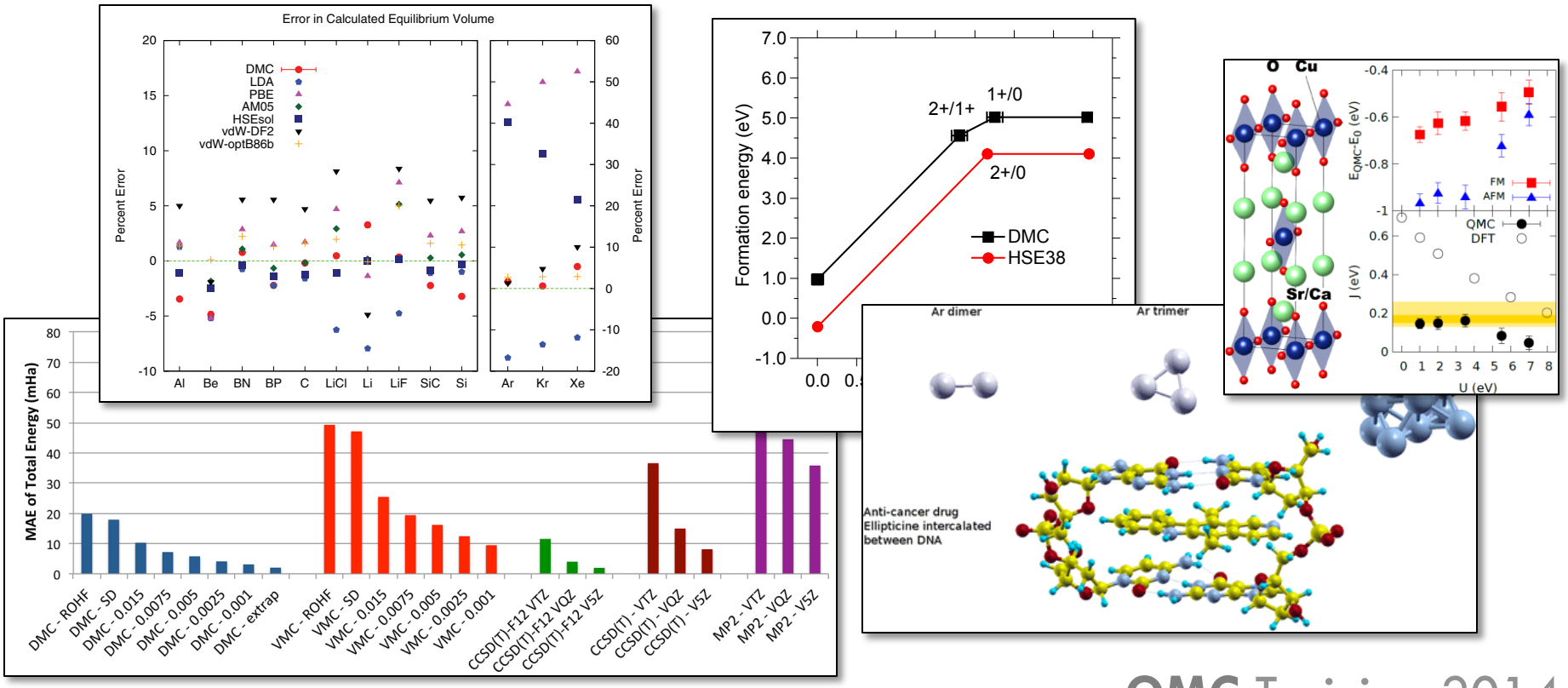
1. Background to **QMC**PACK project
2. Key features
3. Organization: website, releases, planned developments
4. Building QMCPACK
5. Recent science applications

Background

High performance QMC code originally developed at U. Illinois

Open source (BSD license)

Usable for scientific research and competitive publications!



Background

Today, developed by a large number of developers, interested parties

Builds in ~all common computing environments (HPC, clusters, workstations)

C++, Object oriented, extensible, very efficient

MPI Parallelized

Fully OpenMP threaded (important for e.g. large solids by reducing memory usage + increasing efficiency)

GPU CUDA version (currently single determinant, splined wavefunctions)

Standardized XML inputs & HDF5 input/output for large data

Key features

(see website for full details after the training!)

Several flavors of QMC

Variety of wavefunction types

All electron and pseudopotential calculations

Interfaces to Quantum Espresso, GAMESS

Easily extended to other electronic structure codes via standard XML and HDF5 input

e.g. Molpro, NWChem, Qchem, Gaussian, Qbox, abinit…

Analysis tools for minimal environments (perl only) through to python-based with graphs produced via matplotlib ("qmca").

Project suite workflow tool

Project Suite workflow tool

(more Tuesday afternoon, Jaron Krogel)

Flexible python workflow tool

Automation of DFT and QMC calculations (via local job submission, not yet fully distributed.)

Simplified inputs

Provides detailed provenance, improves reproducibility

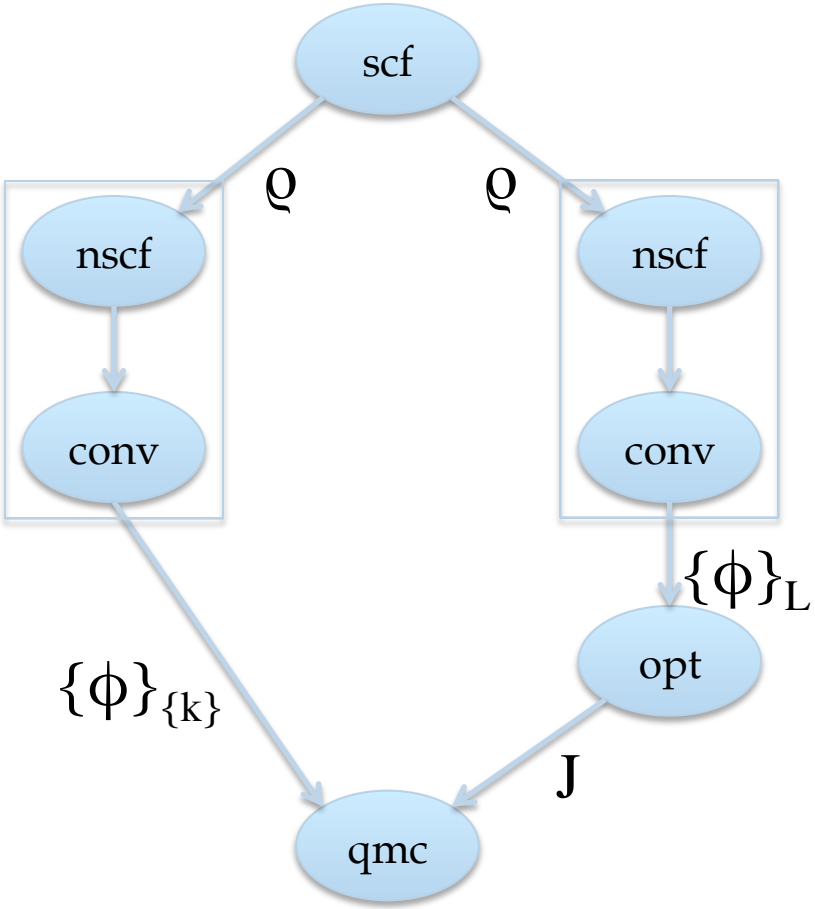
Saves human time, particularly where similar calculations are required for similar systems

Addresses key long term issue in “slowness” of performing QMC calculations

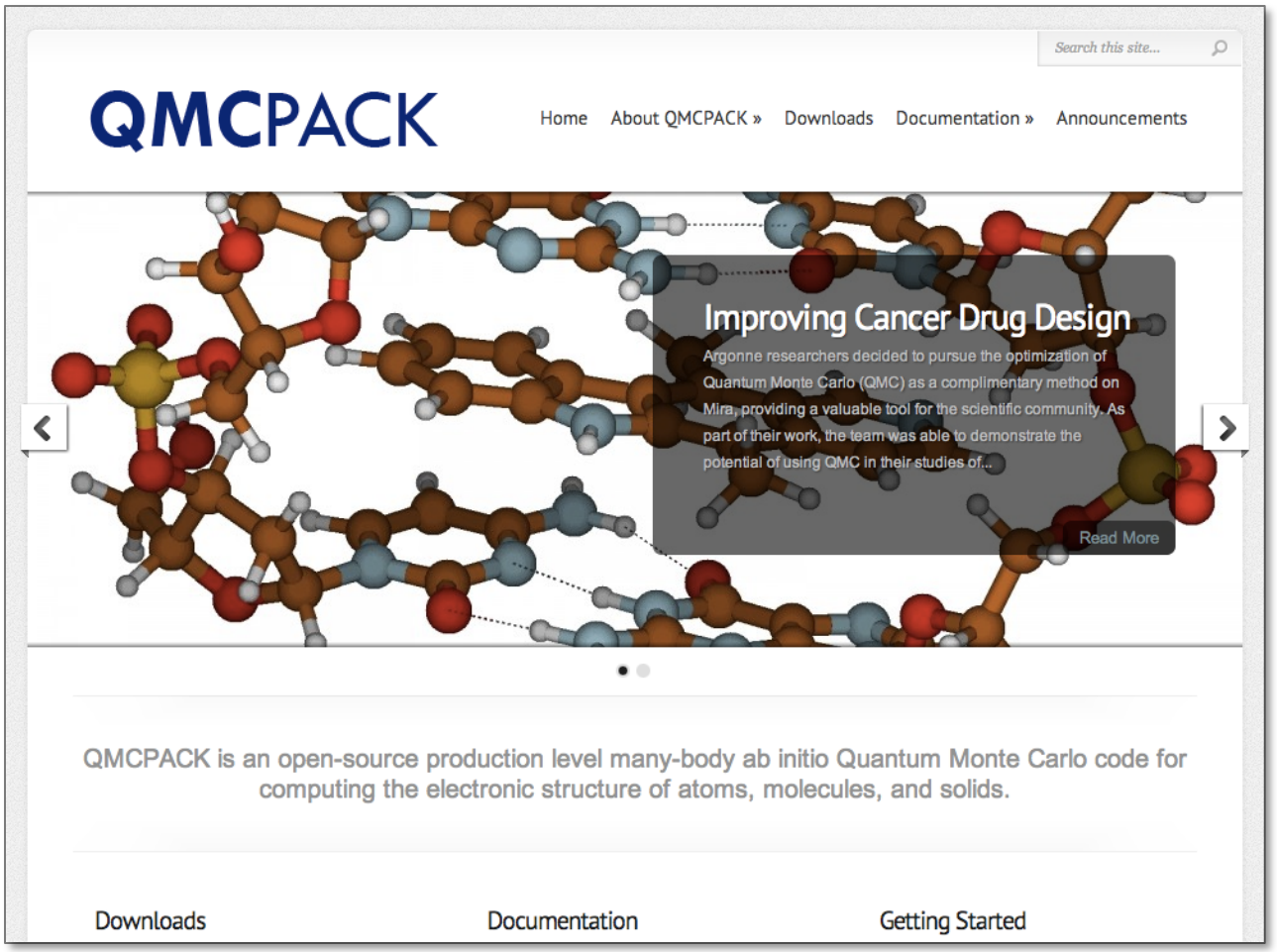
You are still free to run “by hand” — and presently still required to for molecular calculations.

Project Suite workflow tool

Python classes for arbitrary workflows. Sets up input files, runs jobs as a scheduler, analyzes data, passes information to later runs. Straightforward to add additional codes. Very productive because most QMC calculations are small variations on a standard workflow with loops over structures, species, convergence parameters etc.



New website: http://www.qmcpack.org



Beware wet paint! Has only been online a few days.

Material and recordings from this training will migrate to this site

Code releases

Tarballs downloadable on http://www.qmcpack.org

We will maintain a release history

Planning a release every ~6 months or whenever a significant new feature is added (or major bug squashed).

We expect to make updates as a result of feedback from this training.

Planned developments

Easy to run small testsuite to validate your installation

Continuous integration: more extensive test suite to thoroughly validate code, catch build problems on common platforms, test tools etc.

More comprehensive documentation: core features are documented, but (full disclosure!) many features are not.

Developments are prioritized based on perceived importance and your requests

Make suggestions! e.g. Documenting builds on specific HPC machines; new QMC features for particular science applications

Google groups site for discussions

Please post questions, feature requests to

https://groups.google.com/forum/#!forum/qmcpack

Low traffic

Public but posting by membership only (antispam measure)

Preferred to email since others will benefit from reply, but can also directly contact developers

Building QMCPACK

The following is excerpted from the “Getting started” section linked from the documentation section of http://www.qmcpack.org

Building QMCPACK: Dependencies

Ask your system admin / computer center to install these if not already available. Available in most Linux package managers.

C/C++ compiler (recent gnu, Intel…)

cmake, build utility, http://www.cmake.org/

BLAS/LAPACK, numerical library, use platform-optimized libraries

libxml2, XML parser, http://xmlsoft.org/

HDF5, portable I/O library, http://www.hdfgroup.org/HDF5/

Boost, portable C++ source libraries, http://www.boost.org

(Optional) FFTW, FFT library, http://www.fftw.org/

(Optional) doxygen, documentation generator, http://www.doxygen.org

Building QMCPACK

Uses cmake and "out of source" compilation. Similar to autoconfigure scripts - detects features.

```
cd qmcpack
mkdir build
cd build
cmake ..
cmake ..   #note - run cmake twice
make
```

Usually works in standard Linux/UNIX environments. Problems can occur when there are many different compilers available with incompatible libraries etc.

Paul's impression: about as tricky as most DFT codes.

Building QMCPACK

Set environment variables to force use of specific compilers, libraries:

```
export CXX=icpc
export CC=icc
export MKL_HOME=/usr/local/intel/mkl/10.0.3.020
export LIBXML2_HOME=/usr/local
export HDF5_HOME=/usr/local
export BOOST_HOME=/usr/local/boost
export FFTW_HOME=/usr/local/fftw
cmake ..
cmake ..
make
```

Building QMCPACK: **Toolchain files**

QMCPACK is built and run on many different computing systems. Toolchain files provide configurations for specific machines, library locations, compiler versions etc.

Preferred option for building QMCPACK on large systems. Toolchain files are also a valuable starting point for new systems.

```
cd build
cmake -DCMAKE_TOOLCHAIN_FILE=../config/BGQToolchain.cmake ..
cmake -DCMAKE_TOOLCHAIN_FILE=../config/BGQToolchain.cmake ..
make
```

Configurations exist for Titan (OLCF), Blue Waters (NCSA), Rosa (CSCS), Edison (NERSC), generic Linux clusters (w. Intel+MPI)…

Known limitation: Currently OS X does not build successfully, but seems very close (macports)

Advice: Try on a completely standard system first!

Applications

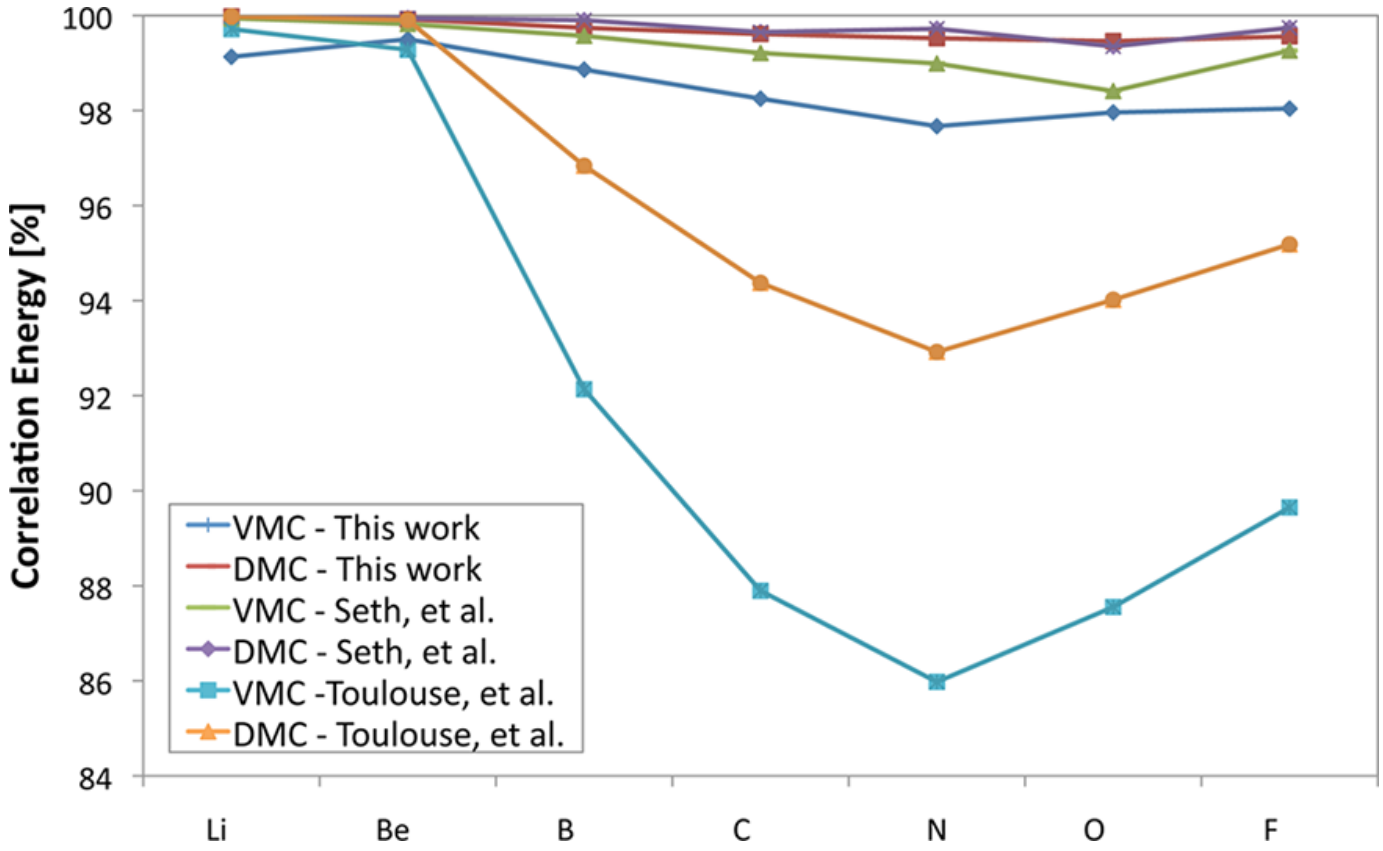
& Recommended Reading!

Important: Many other valuable QMC works have been published by other groups – this small selection concentrates on **QMC**PACK-related works & is not comprehensive

Benchmarking the accuracy of QMC for molecules

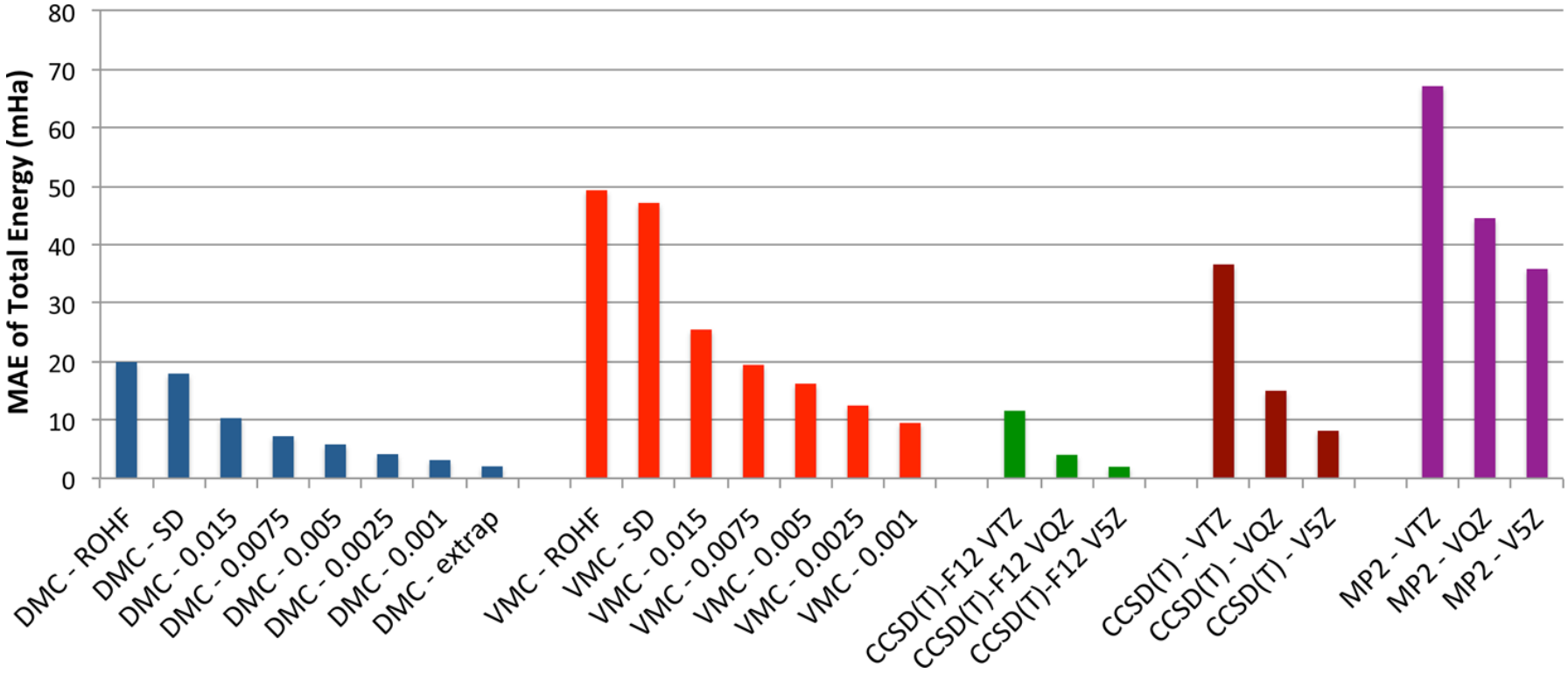
"Multideterminant Wave Functions in Quantum Monte Carlo", M. A. Morales, …, G.E.Scuseria. JCTC **8** 2182 (2012) http://dx.doi.org/10.1021/ct3003404

High accuracy achievable for atoms:



Benchmarking the accuracy of QMC for molecules

Testing accuracy for G1 test set (C_2H_2, CN, H_2O, NaCl,SiH_4, SiO...), going beyond single determinant "standard recipe". MAE of 0.8kcal/mol achieved for atomization energies, i.e. Chemical accuracy.

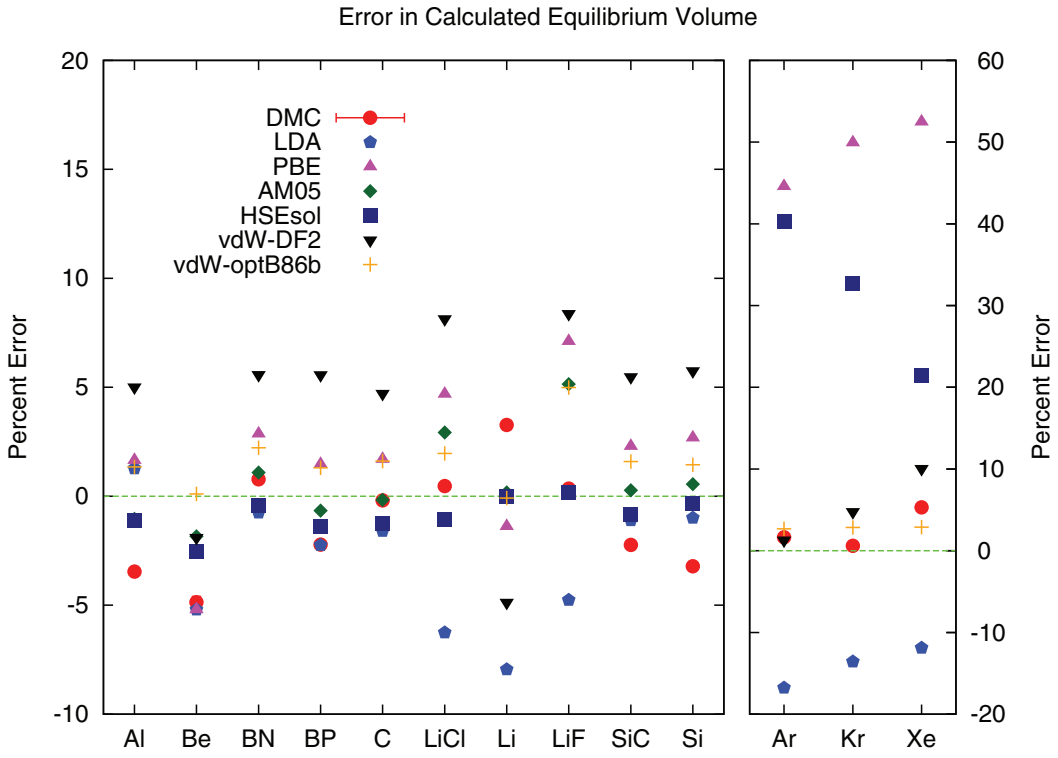


See also Nemec et al. JCP **132** 034111(2010) http://dx.doi.org/10.1063/1.3288054 all electron single determinant tests for same test set (CASINO code).

Benchmarking the accuracy of QMC for solids

Analysis of structural properties (V, B_0) of ionic, metallic, covalent and van der Waals solids using "standard recipe" single determinant Slater-Jastrow pseudopotentials. Careful convergence of calculations. Finds high accuracy over whole set of solids.

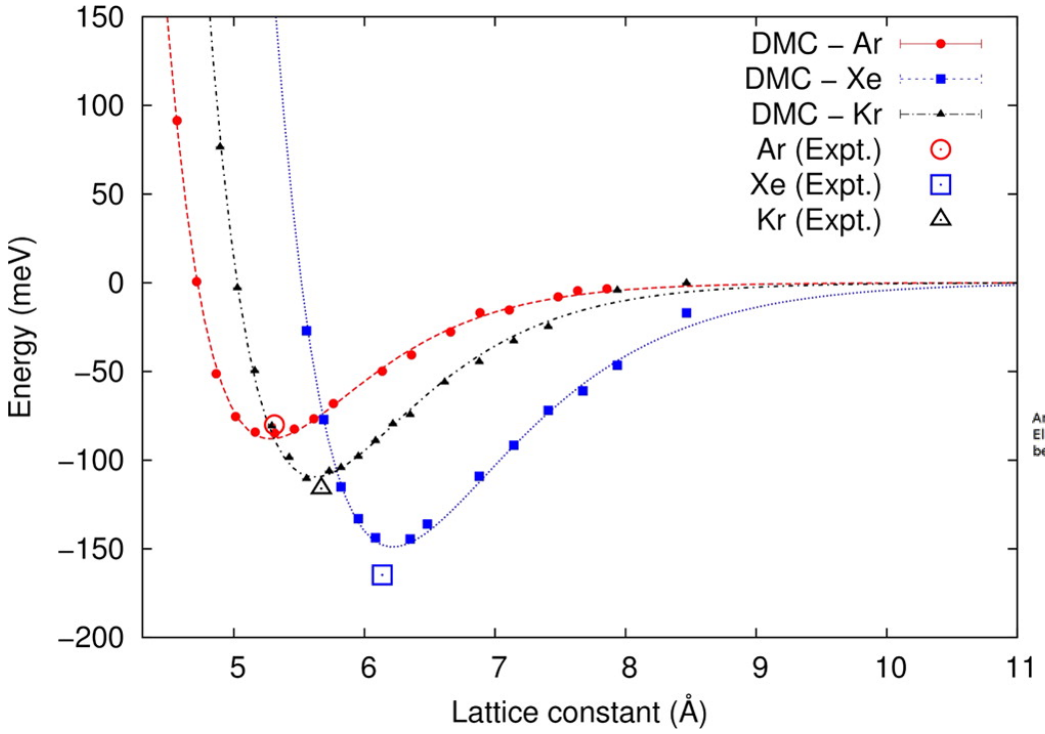
"Quantum Monte Carlo applied to solids" L. Shulenburger & T. R. Mattsson PRB **88** 245117 (2013) http://dx.doi.org/10.1103/PhysRevB.88.245117 Editors' Suggestion.

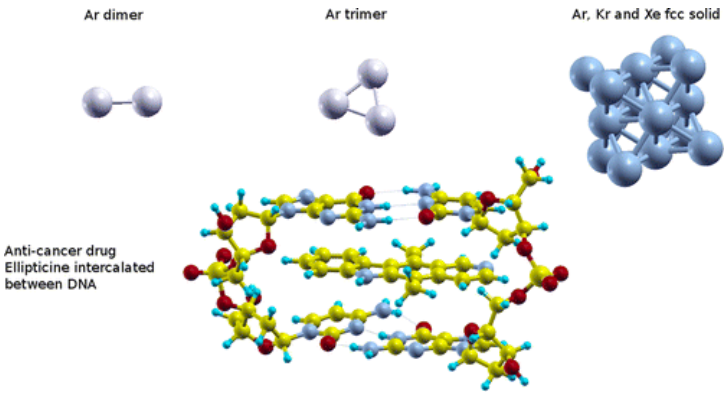


van der Waals interactions

Extensive DMC calculations for noble gas solids, clusters and DNA+intercalating drug molecule. Drug molecule requires 3 body corrections in vdw DFT to ~match DMC results, while some other correction schemes overbind. (PBE DFT does not bind)

A. Benali, L. Shulenberger, N. A. Romero, J. Kim, O. Anatole von Lilienfeld JCTC (June 2014), http://dx.doi.org/10.1021/ct5003225

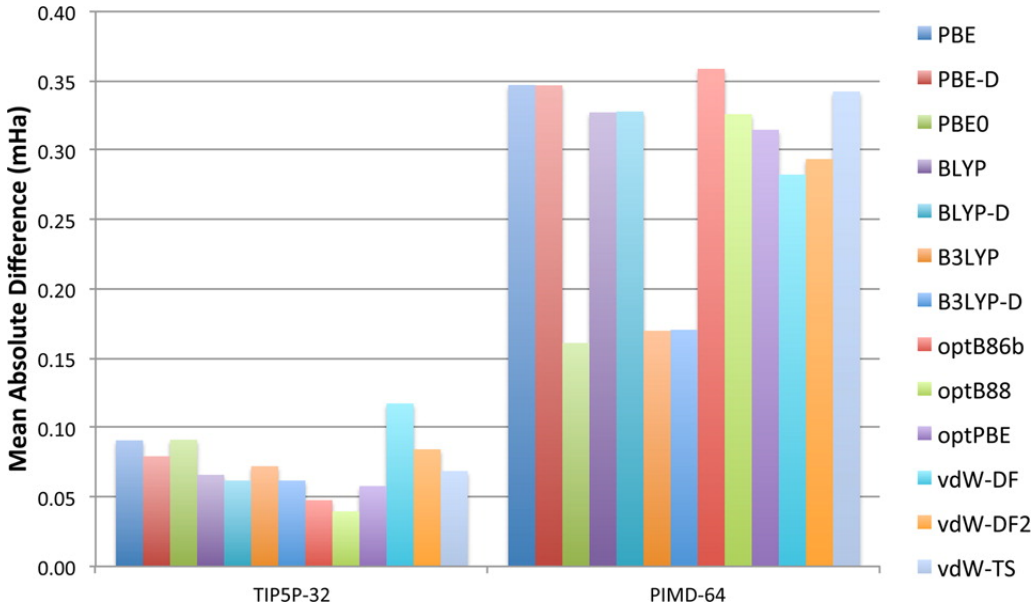




Benchmarking density functionals for bulk water

M. A. Morales, J. R. Gergely, J. McMinis, J. M. McMahon, J. Kim, and D. M. Ceperley
JCTC 10 2355 (2014) http://dx.doi.org/10.1021/ct500129p

Analysis of energies of water configurations taken from TIP5P and PIMD (path integral) simulations computed using various DFT functionals vs DMC. Identifies a possible route to optimizing functionals for specific applied problems.

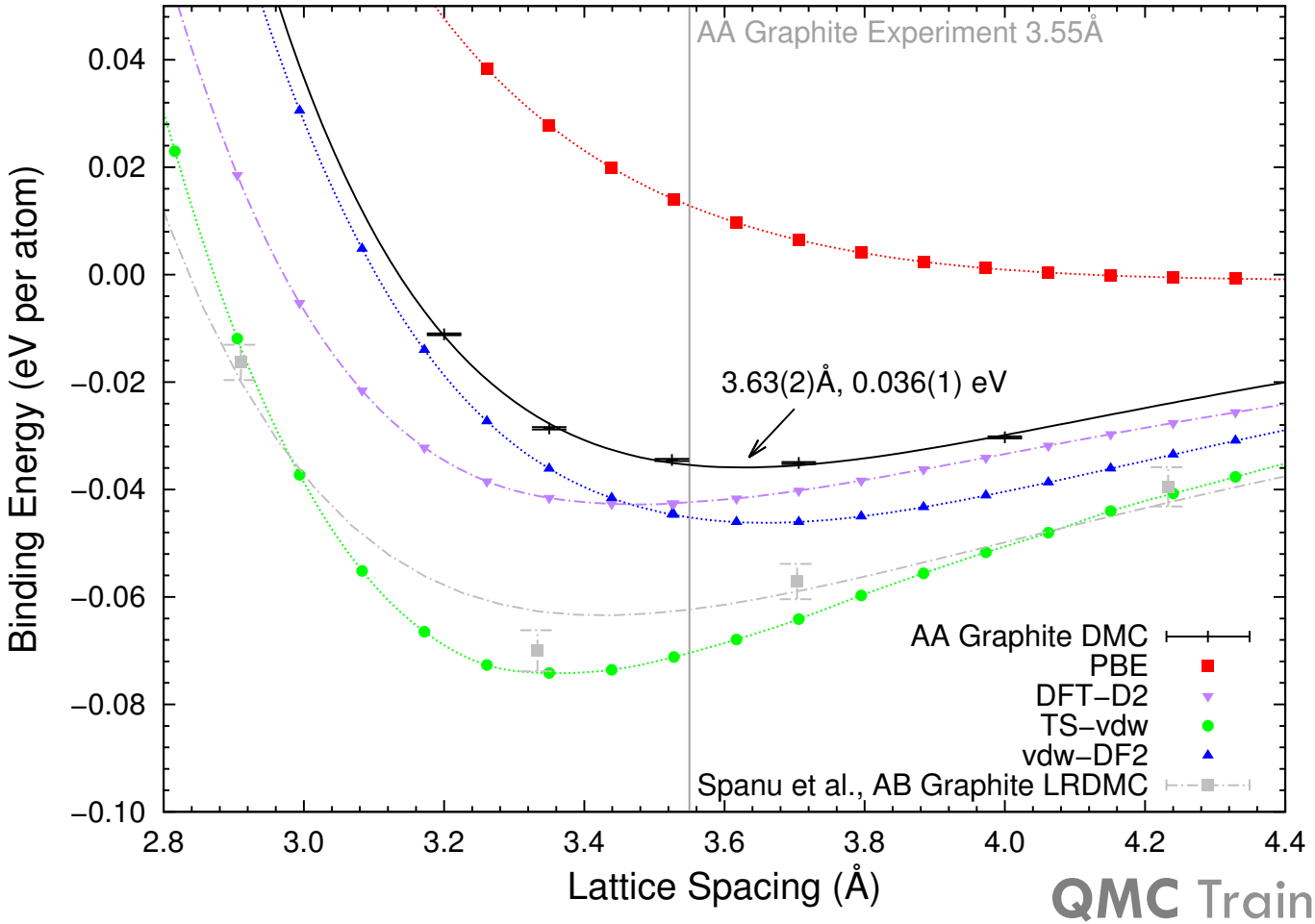


"We found that, while optB88 seems to provide the best description of dispersion in the liquid, the vdW-DF and vdW-DF2 functionals offer the best agreement of all nonhybrid functionals when fully flexible, realistic water configurations are considered."

Binding and diffusion of lithium in graphite

DMC calculations accurately predict the lattice constant and binding energy of A-A graphite relative to A-B graphite. When dilute Li is added, self-consistent van der Waals DFTs outperform empirical schemes due to the importance of charge transfer.

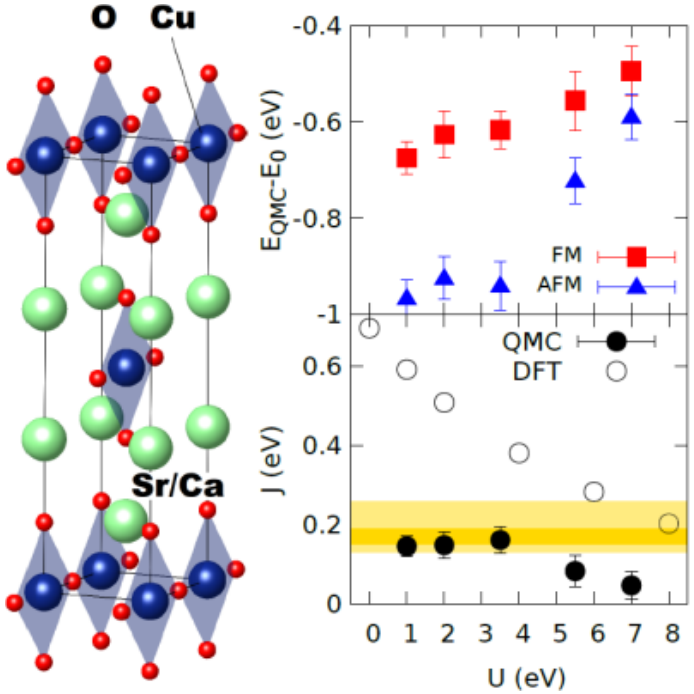
P. Ganesh, J. Kim, C. Park, M. Yoon, F. A. Reboredo, and P. R. C. Kent (submitted).



Computing the exchange constant in cuprates

Within a variational scheme (a non-empirical scheme), DMC predicts exchange constants in good agreement with experiment for Ca_2CuO_3. Indicates promise for describing ground state properties of strongly correlated materials.

K. Foyevtsova, J. T. Krogel, J. Kim, P. R. C. Kent, E. Dagotto, F. A. Reboredo. Accepted in PRX (2014) and http://arxiv.org/abs/1402.5561

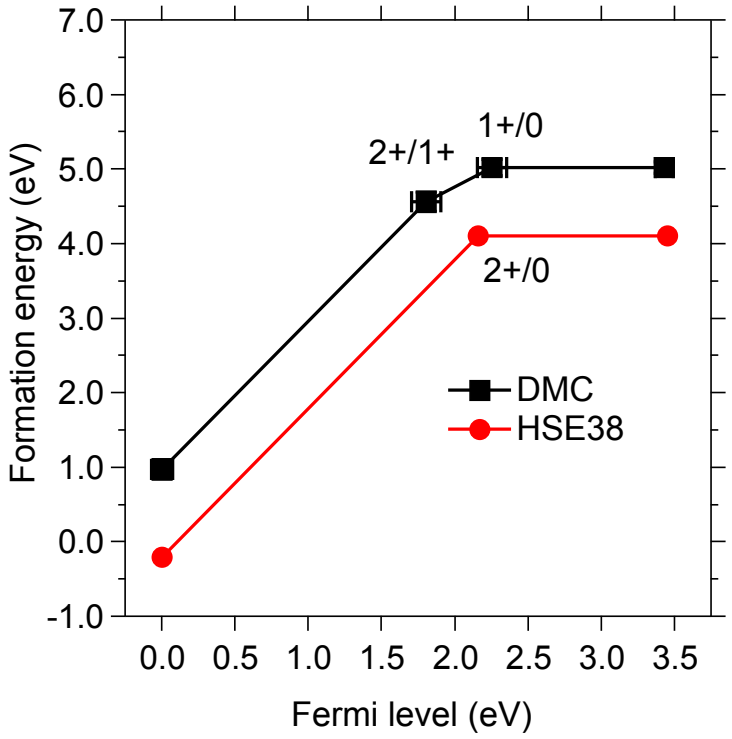


Also see QMC results for La_2CuO_4, with more properties considered including phonons, L. Wagner & P. Abbamonte http://arxiv.org/abs/1402.4680

The vacancy in ZnO

DMC calculations rule out the oxygen vacancy as the source of persistent n-type conductivity in ZnO. Confirms previous DFT predictions but finds (i) much higher oxygen vacancy formation energy that HSE or other DFT approximations, (ii) finds a positive U behavior in contrast to the DFT.

"Ab initio many-body calculations of the oxygen vacancy in ZnO", J. A. Santana, J. T. Krogel, J. Kim, P. R. C. Kent, and F. A. Reboredo, http://arxiv.org/abs/1406.3169



Summary

QMCPACK is a full featured QMC code usable for production scientific investigations

There is a new website qmcpack.org, documentation, and project coordination

Improvements in the code, documentation, features etc. will be based on perceived need and feedback received. Be vocal!

Questions?